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Anharmonic Phonon Behavior in BCC Iron at High Temperatures

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The phonon density of states (DOS) of bcc ⁵⁷Fe was measured from 300 K to 1223 K using nuclear resonant inelastic x-ray scattering. All phonons shift to lower energies (soften) with temperature. The different phonons soften in a similar way, at least below the Curie temperature of 1043K. At temperatures above the Curie temperature, the low transverse modes soften more rapidly. Interatomic force constants for the bcc phase were obtained by iteratively fitting a Born von-Karman model to the experimental phonon spectra. Trends in these force constants are used to interpret the thermal softening of the different phonons. The unusually large phonon anharmonicity of bcc Fe at elevated temperatures is discussed in terms of the temperature dependences of the first and second-neighbor interatomic force constants.